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THE INFLUENCE OF COMPUTER ARCHITECTURES

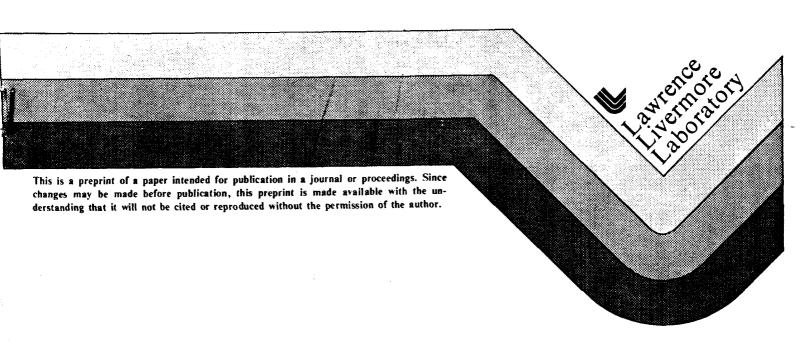
ON NUMERICAL ALGORITHMS

by

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Workshop on High Speed Computing Gleneden Beach, Oregon

March 31, 1981



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THE INFLUENCE OF COMPUTER ARCHITECTURES

ON

NUMERICAL ALGORITHMS

BY

GARRY RODRIGUE

COMPUTER RESEARCH GROUP

LAWRENCE LIVERMORE NATIONAL LABORATORY

IN THIS TALK,

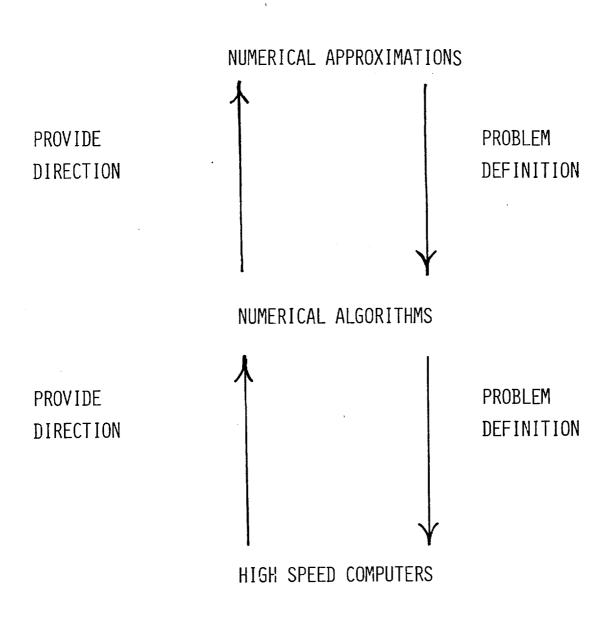
- 1) AREAS THAT EFFECT NUMERICAL ALGORITHMS
- 2) HOW THESE AREAS EFFECT NUMERICAL ALGORITHMS
- 3) SHOW EXAMPLES OF HOW COMPUTERS HAVE INFLUENCED NUMERICAL ALGORITHMS BOTH IN THE PAST AND THE PRESENT
- 4) DISCUSS SOME OF THE DIFFICULTIES DEVELOPING NUMERICAL ALGORITHMS

AREAS THAT EFFECT NUMERICAL ALGORITHMS

THE NUMERICAL PROCESS IN SCIENCE

SCIENCE PROBLEM		NEUTRON TRANSPORT FLUID FLOW
MATH. MODEL		BOLTZMANN EQTN. NAVIER-STOKES EQTNS.
MATH. APPROX.		DIFFUSION INVISCID FLOW
NUM. APPROX.		BACKWARD EULER FORMULA LAX-WENDROFF FORMULA
₩ NUM. ALG. I		TRIDIAGONAL MATRIX SOLVER
COMPUTER		CDC-7600 CRAY-1

HOW THESE AREAS INFLUENCE NUMERICAL ALGORITHM

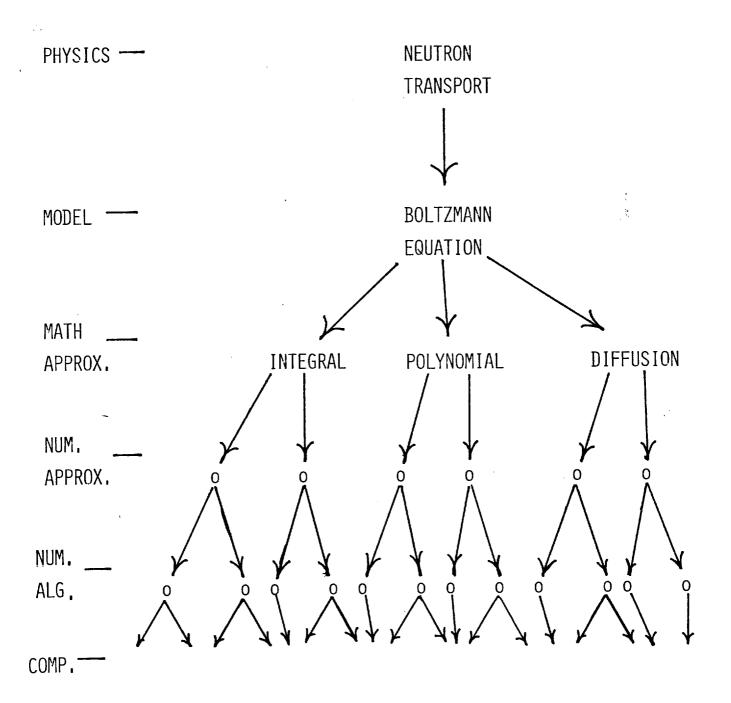


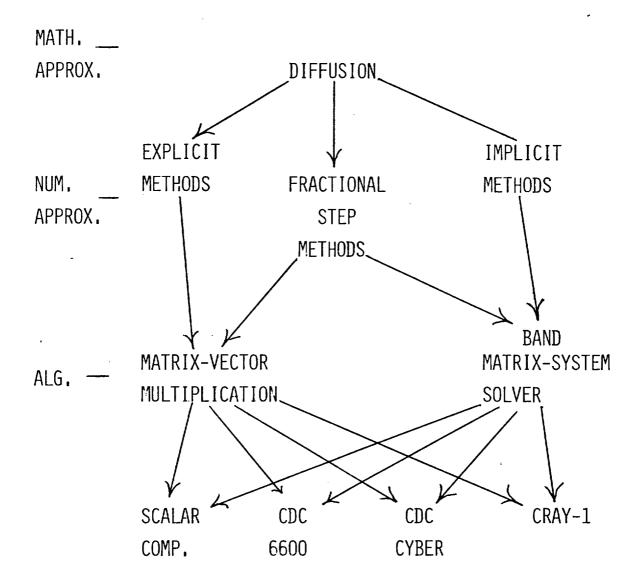
FOCUS ON ALGORITHMS FOR MATRIX CALCULATIONS

SPECIFICALLY:

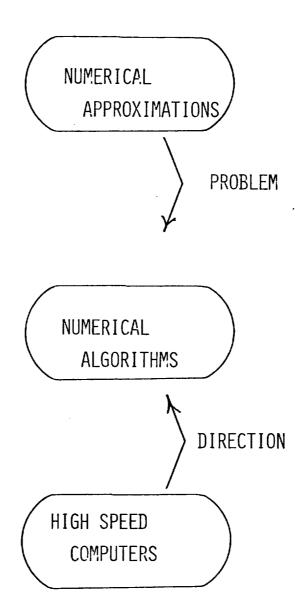
- 1) MATRIX-VECTOR MULTIPLICATION ALGORITHM
- 2) BANDED MATRIX INVERSION ALGORITHM

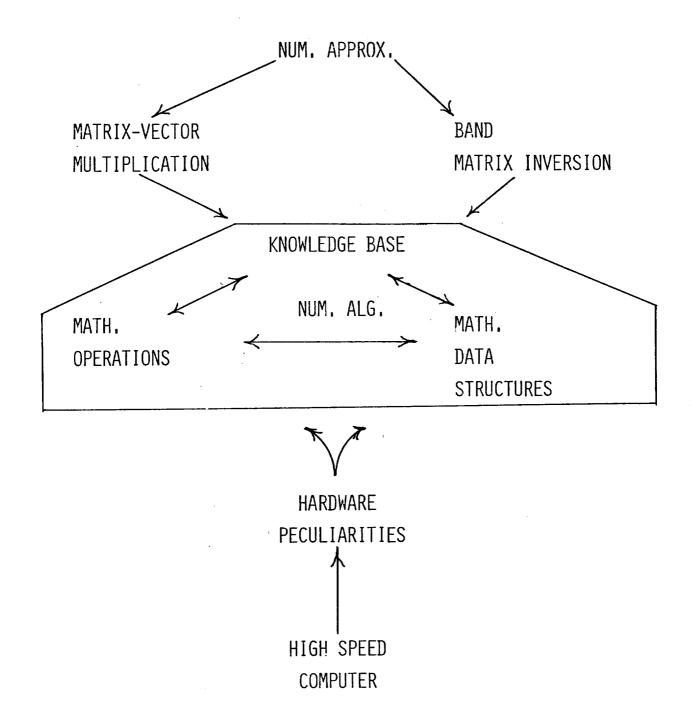
MATRIX ALGORITHMS ARE IMPORTANT FOR PERFORMING TRANSPORT CALCULATIONS:



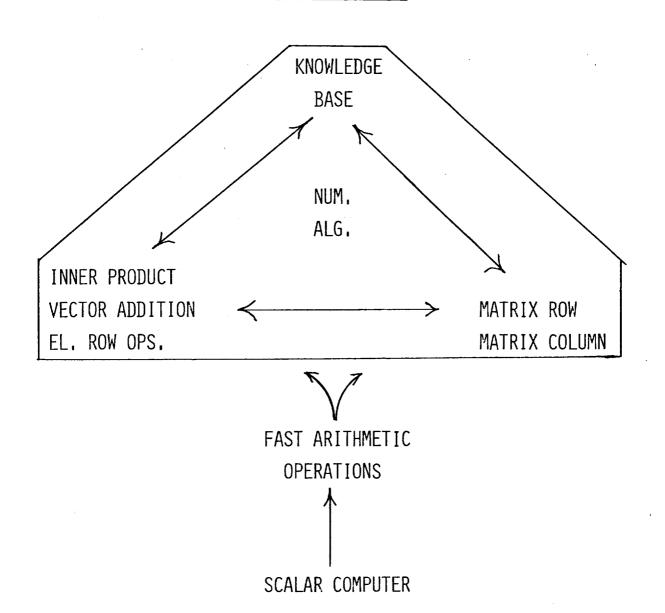


RECALL:





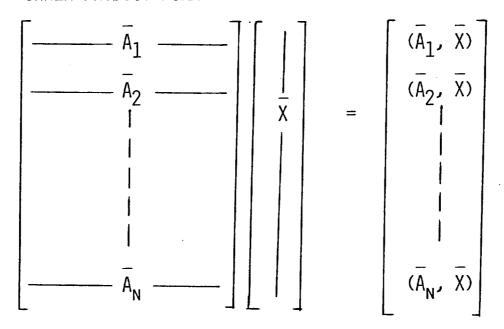
AS AN EXAMPLE, LET US FIRST GO BACK TO THE "SCALAR ERA" TO SEE HOW MATRIX ALGORITHMS WERE DEVELOPED



$$\begin{bmatrix} A_{11}X_1 & + & A_{12}X_2 & +----+ & A_{1N}X_N \\ A_{21}X_1 & + & A_{22}X_2 & +---+ & A_{2N}X_N \\ & & & & & & & & \\ & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & &$$

MATRIX-VECTOR MULTIPLICATION ALGORITHMS

• INNER PRODUCT FORM



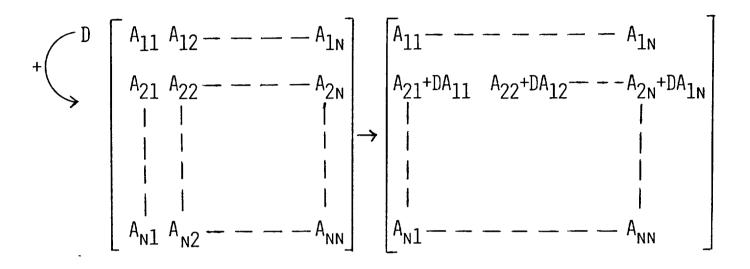
OUTER PRODUCT FORM

$$\begin{bmatrix} \frac{1}{A_{1}} & \frac{1}{A_{2}} & - & - & \frac{1}{A_{N}} \end{bmatrix} \begin{bmatrix} x_{1} \\ x_{2} \\ \vdots \\ x_{N} \end{bmatrix} = A_{1} x_{1} + A_{2} x_{2} + \cdots + A_{N} x_{N}$$

WITHOUT GOING INTO TOO MUCH DETAIL, THESE FORMS OF MATRIX MULTIPLICATION LED TO DEVELOPMENT OF MANY NEW ALGORITHMS.

- 1) CONJUGATE GRADIENT METHODS
- 2) HOUSEHOLDER METHODS
- 3) QR AND QZ METHODS
- 4) POWER AND DEFLATION METHODS
- 5) VARIABLE METRIC METHODS

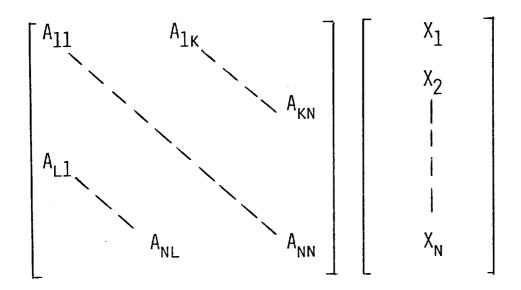
ELEMENTARY ROW OPERATION



LED TO DEVELOPMENT OF

- VARIANTS OF GAUSS ELIMINATION ALGORITHM
- 2) FACTORIZATION ALGORITHMS
- 3) GIVENS ALGORITHM

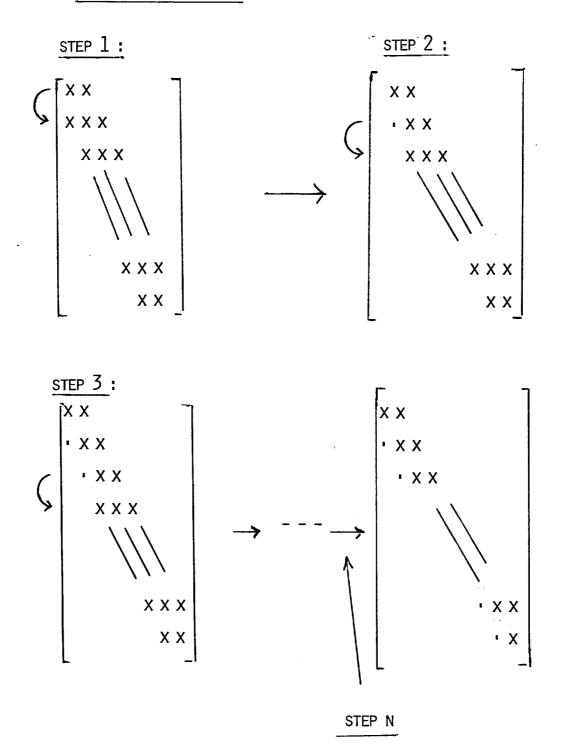
BANDED MATRICES



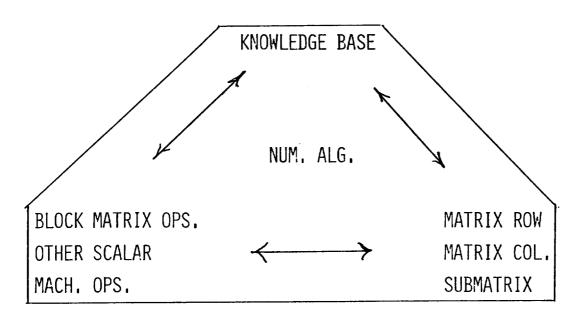
- FOR SCALAR MACHINES, ALGORITHMS DEVELOPED USING ROW AND COLUMN OPERATIONS WENT FASTER FOR BANDED SYSTEMS

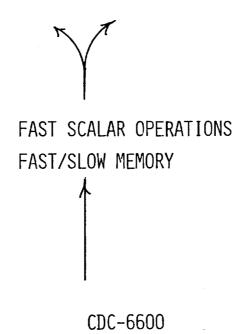
THE CLASSICAL ALGORITHM IS GAUSSIAN ELIMINATION

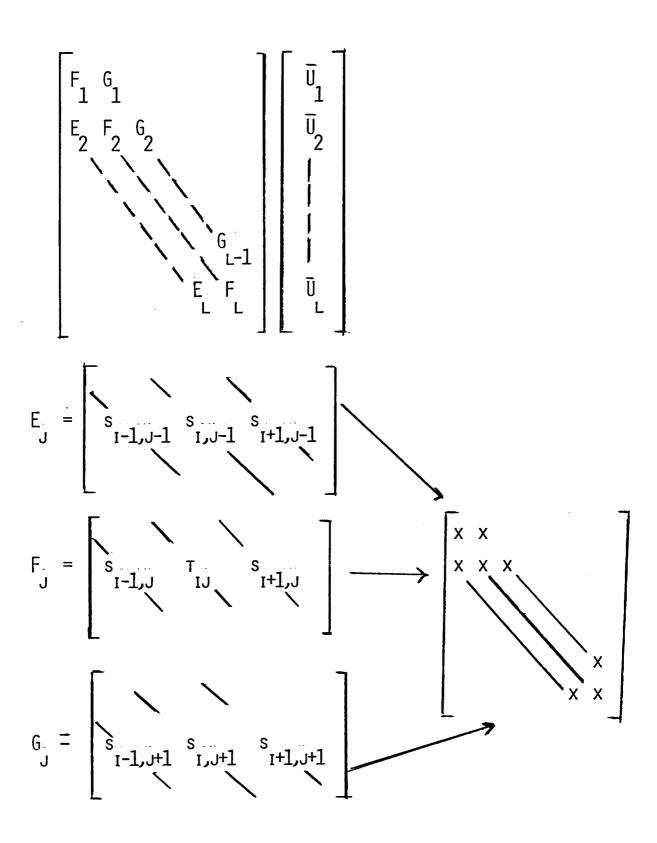
- FORWARD SUBSTITUTION



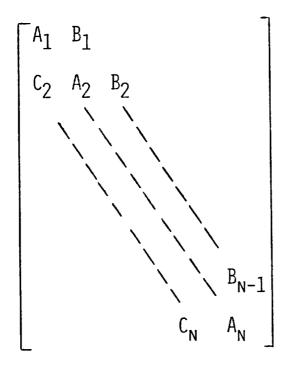
FAST/SLOW MEMORY MACHINES







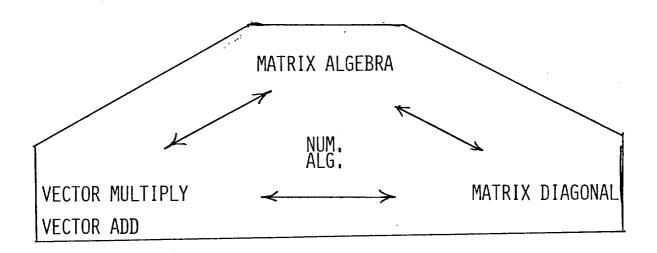
EFFICIENT ALGORITHMS WERE THOSE THAT COULD MANIPULATE THE BLOCKS OF THE MATRIX EFFECTIVELY

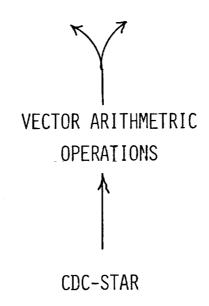


 A_{1} , B_{1} , C_{1} ARE MATRICES

- LED TO DEVELOPMENT OF
 - 1) BLOCK ITERATIVE METHODS
 - 2) FAST POISSON/BIHARMONIC SOLVERS
 - 3) COMPANION MATRIX ALGORITHMS

CDC-STAR





CONSTRAINTS OF THE STAR

- 1) SLOW SCALAR ARITHMETIC OPERATIONS
- 2) SLOW VECTOR INSTRUCTIONS WHEN VECTORS ARE SHORT

1) SCALAR X VECTOR

$$A \begin{bmatrix} X_1 \\ X_2 \\ I \\ I \\ X_N \end{bmatrix} = \begin{bmatrix} AX_1 \\ AX_2 \\ I \\ I \\ AX_N \end{bmatrix}$$

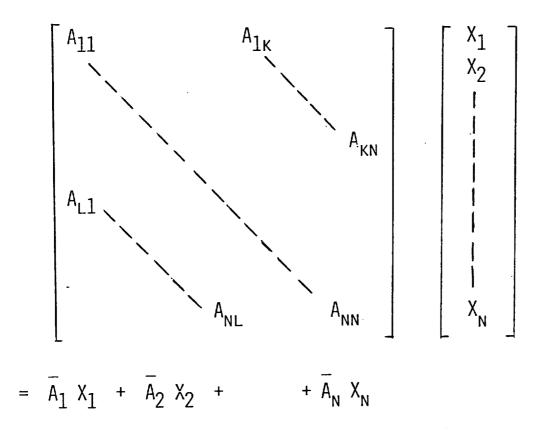
2) VECTOR ADDITION

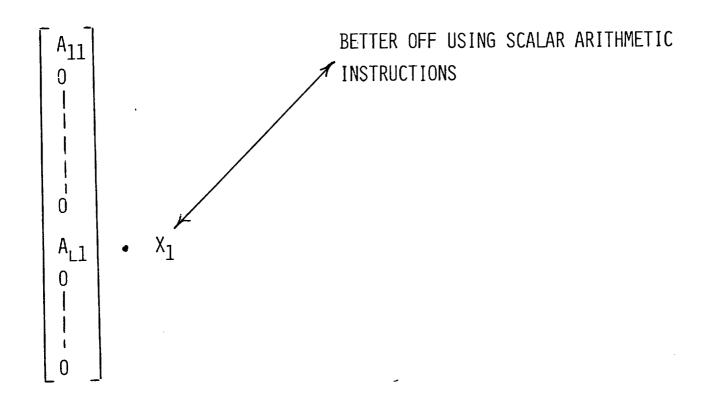
3) VECTOR MULTIPLICATION**

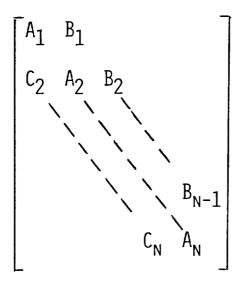
MATRIX-VECTOR MULTIPLICATION

$$\begin{bmatrix}
- & \overline{A}_{1} - & \overline{A}_{2} - & \overline{A}_{2} - & \overline{A}_{2} - & \overline{A}_{N} - & \overline{A}_{N} - & \overline{A}_{N}
\end{bmatrix} = \begin{bmatrix}
\overline{A}_{1}, \overline{X} \\ \overline{A}_{2}, \overline{X} \\ \overline{X} \\ \overline{A}_{N}, \overline{X}
\end{bmatrix} = \begin{bmatrix}
\overline{A}_{1}, \overline{X} \\ \overline{A}_{2}, \overline{X} \\ \overline{A}_{N}, \overline{X}
\end{bmatrix}$$

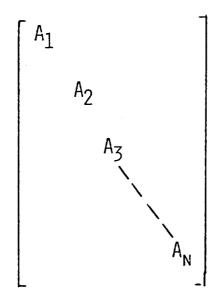
WHAT HAPPENS ON A BANDED MATRIX?

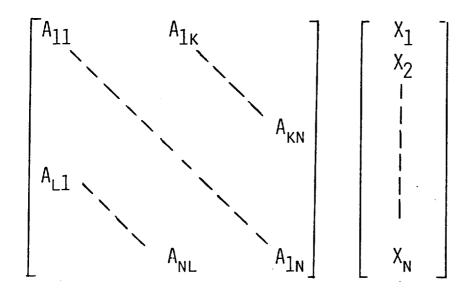




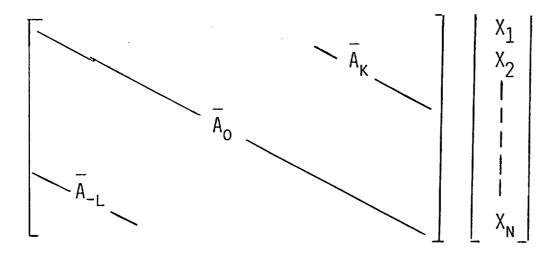


 ALGORITHMS DERIVED USING BLOCK STRUCTURES RESULTED IN SHORT VECTORS





IN VECTOR NOTATION



$$\equiv \overline{A}_{0} \quad \begin{bmatrix} X_{1} \\ X_{2} \\ \vdots \\ X_{N} \end{bmatrix} \quad ---- \quad \begin{bmatrix} X_{1} \\ \vdots \\ X_{N} \end{bmatrix} \quad + \overline{A}_{K} \quad \begin{bmatrix} X_{1} \\ \vdots \\ X_{N} \end{bmatrix}$$

- GENERALIZATION TO MORE COMPLICATED SYSTEMS IS EASY

GENERAL COMMENTS

DIAGONAL ALGORITHM IS

30 - 40 TIMES FASTER ON STAR-100

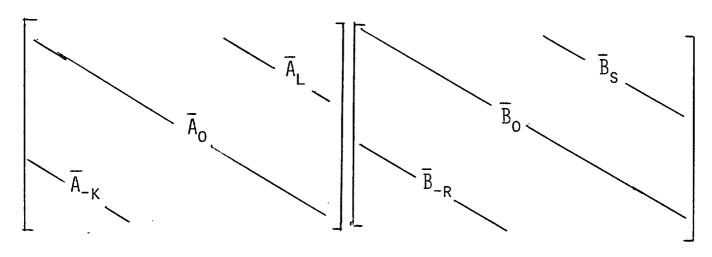
5 - 8 TIMES FASTER ON CRAY-1

THAN CLASSICAL ROW AND COLUMN ALGORITHM

- NO MATHEMATICAL OR GEOMETRICAL THEORY OF MATRIX-VECTOR ALGORITHM USING DIAGONALS AS A VECTOR STRUCTURE HAS EVER BEEN CARRIED OUT.
- WE NEED THIS IF MORE EFFICIENT ALGORITHMS FOR VECTOR OR MULTI-PROCESSING MACHINES ARE TO BE INVENTED.

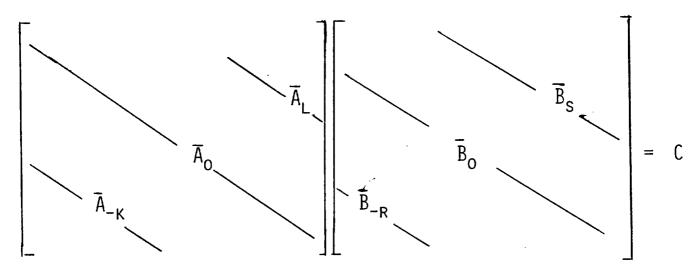
AN EXAMPLE OF HOW RESULTS USING DIAGONAL VECTORS CAN LEAD TO NEW ALGORITHMS

- MATRIX MULTIPLICATION: AB = C



$$= \begin{bmatrix} \bar{c}_0 & \bar{c}_1 \\ \bar{c}_{-1} \end{bmatrix}$$

 $\frac{\text{RESULT 1:}}{\text{DIAGONALS \overline{A}_I AND \overline{B}_J ARE NON-ZERO, THEN}} \\ = \frac{1}{1} \frac$

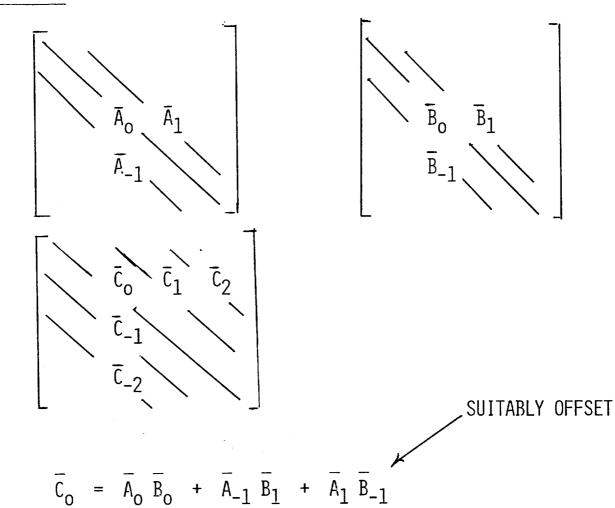


• NON-ZERO DIAGONALS OF C

\bar{c}_{o}	C-K
_ C _{-K-R}	\overline{C}_L
_ C_ _{K+S}	\overline{C}_{-R}
\overline{C}_{L-R}	\overline{c}_s
\bar{C}_{L+S}	

RESULT 2: THE PRODUCT \overline{A}_I \overline{B}_J CONTRIBUTES TO THE FORMATION OF \overline{C}_{I+J}

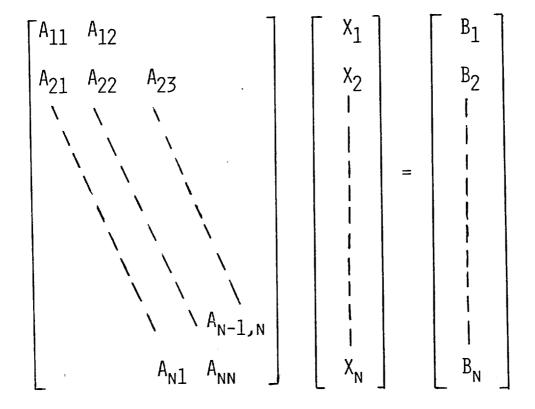
EXAMPLE



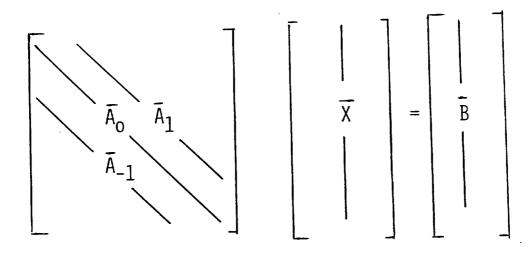
I.E., EACH DIAGONAL CAN BE CONSTRUCTED FROM VECTOR
PRODUCTS AND ADDITIONS

WE USE THESE TWO RESULTS TO GENERATE AN ALGORITHM TO SOLVE A TRIDIAGONAL SYSTEM OF EQUATIONS

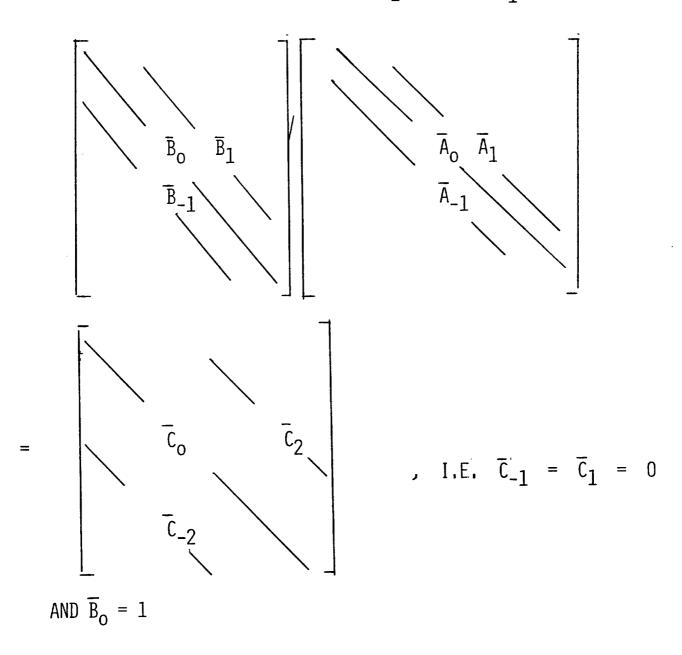
PROBLEM STATEMENT: TX = B



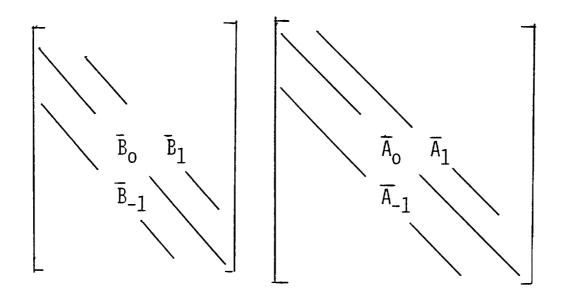
DIAGONAL FORM



CONSTRUCT TRIDIAGONAL MATRIX Q_1 SO THAT: Q_1 T =



PROCEDURE

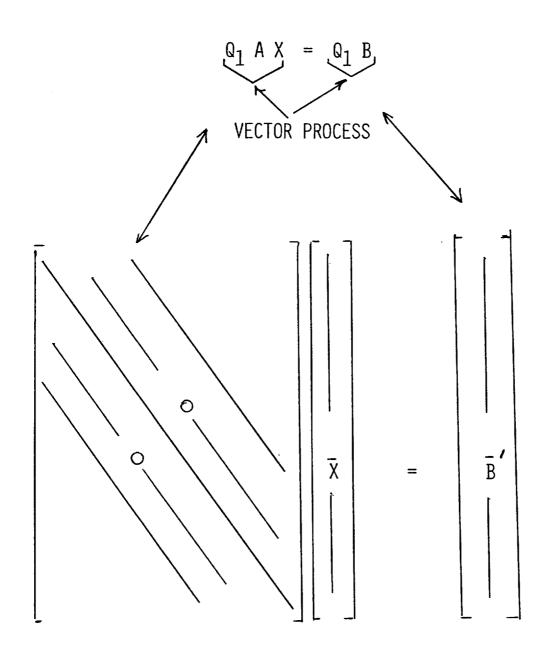


ANALYSIS: FROM RESULTS 1 AND 2,

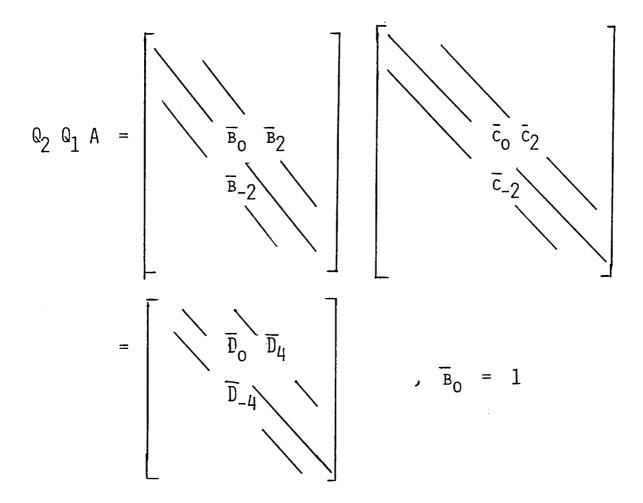
$$\overline{B}_0 \overline{A}_1 + \overline{B}_1 \overline{A}_0 = \overline{C}_1 = 0$$
 $\overline{B}_0 \overline{A}_{-1} + \overline{B}_{-1} \overline{A}_0 = \overline{C}_{-1} = 0$

BUT
$$\overline{B}_{O} = 1$$
:
$$\overline{B}_{1} = -\overline{A}_{1}/\overline{A}_{O}$$

$$\overline{B}_{-1} = -\overline{A}_{-1}/\overline{A}_{O}$$

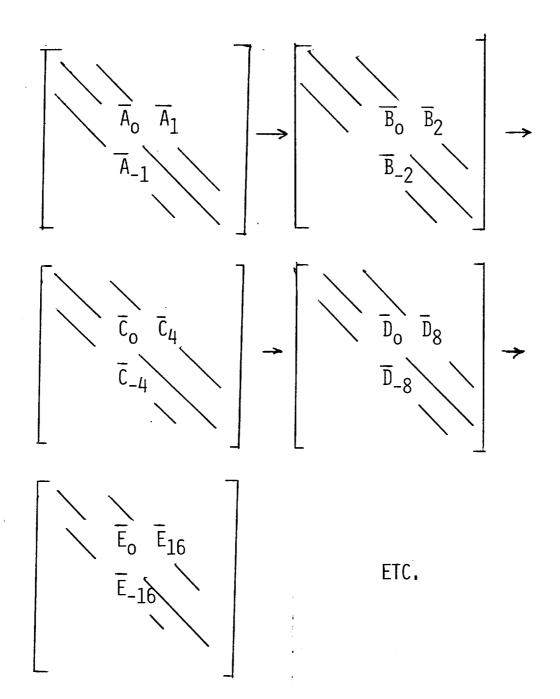


STEP 2: CONSTRUCT MATRIX \mathbf{Q}_2 SO THAT



- CONSTRUCT
$$Q_2$$
 AS BEFORE: $\overline{B}_{-2} = -\overline{A}_{-2}/\overline{A}_0$

$$\overline{B}_2 = -\overline{A}_2/\overline{A}_0$$



OTHER VECTOR ALGORITHMS CAN BE GENERATED WITH THIS PROCEDURE

- RECURSIVE DOUBLING
- ODD-EVEN REDUCTION
- PARALLEL GAUSS ELIMINATION
- CYCLIC REDUCTION**

AFTER $LOG_2N = M$ STEPS:

$$Q_{M} Q_{M-1} . . . Q_{1} A \overline{X} = \begin{bmatrix} \overline{Z}_{0} & \overline{X} \\ \overline{X} & \overline{X} \end{bmatrix}$$

$$= Q_{M} Q_{M-1} . . . Q_{1} \overline{B}$$

$$= \overline{B}'$$

FINAL SOLUTION:

$$\bar{X} = \bar{B}' / \bar{Z}_0$$

CYCLIC REDUCTION vs. RECURSIVE DOUBLING

STEPS

BOTH REQUIRE LOG2N STEPS

AVERAGE VECTOR LENGTHS

RECURSIVE DOUBLING: $N - 2^{\kappa-1}$

CYCLIC REDUCTION: N/2K

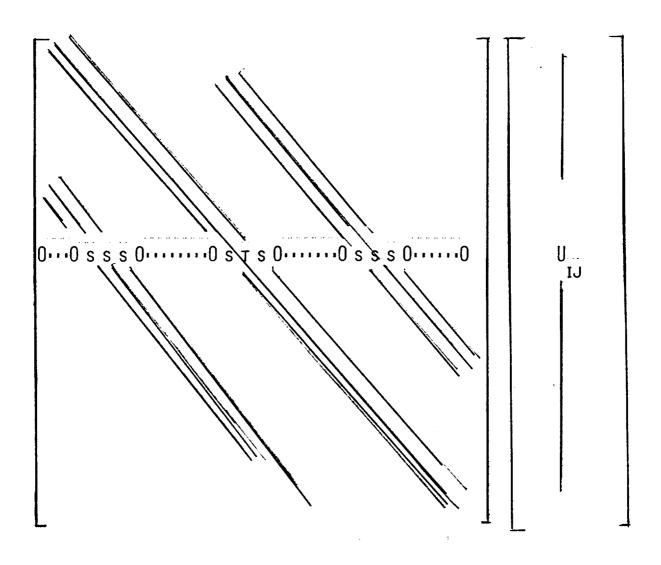
COMPLEXITY

RECURSIVE DOUBLING: EASY TO CODE, EASY TO

UNDERSTAND

CYCLIC REDUCTION: DIFFICULT TO CODE, DIFFICULT

TO UNDERSTAND

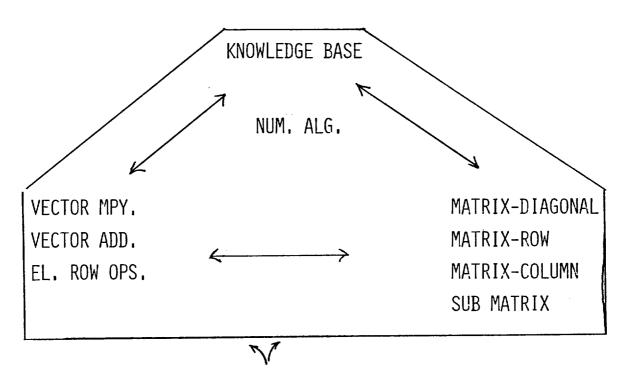


OPTIMAL ALGORITHMS FOR VECTOR PROCESSORS

- OPTIMAL ALGORITHMS WILL USE
 - COLUMN VECTOR OPERATIONS
 - ROW VECTOR OPERATIONS
 - DIAGONAL VECTOR OPERATIONS

IN AN EFFICIENT MANNER

- EG. WHEN VECTORS (I.E. DIAGONALS) BECOME TOO SHORT,
SWITCH TO ROW OR COLUMN VECTOR OPERATIONS TO CREATE
ALGORITHM



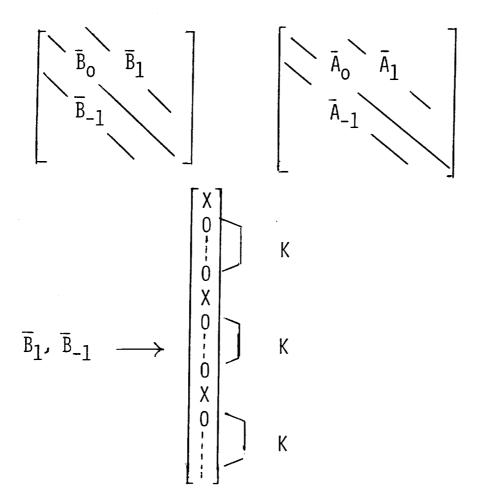
SCALAR ARITH, OPS.

VECTOR OPS.

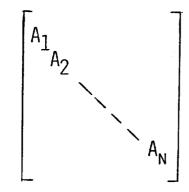
NON-CONTIGUOUS VEC. OPS.



EFFICIENT MATRIX-MULTIPLICATION ALGORITHMS BY NON-CONTIGUOUS DIAGONAL VECTORS (EVENLY INCREMENTED) WAS NOW POSSIBLE



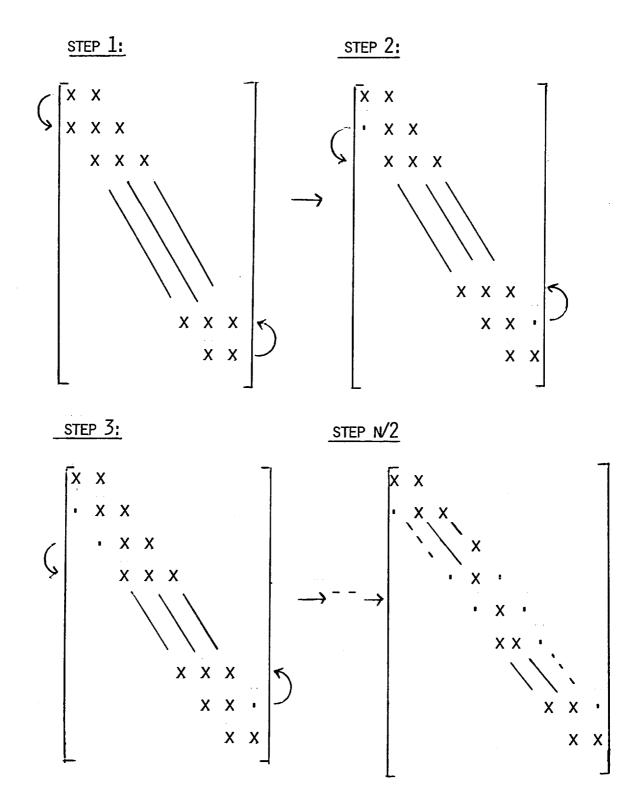
NOW CAN HANDLE



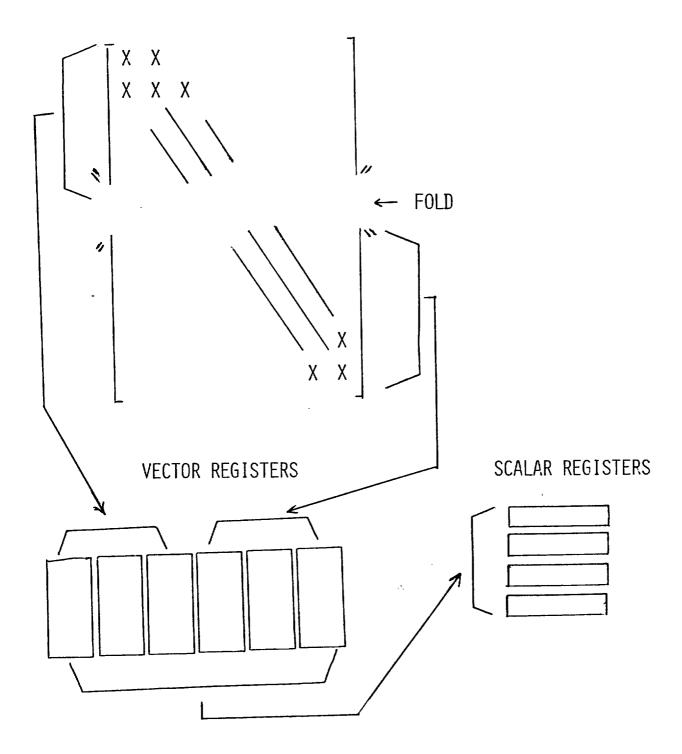
LEADS TO VARIANTS OF CYCLIE REDUCTION ALG.

THE FOLDING ALGORITHM

(FORWARD SUBSTITUTION)

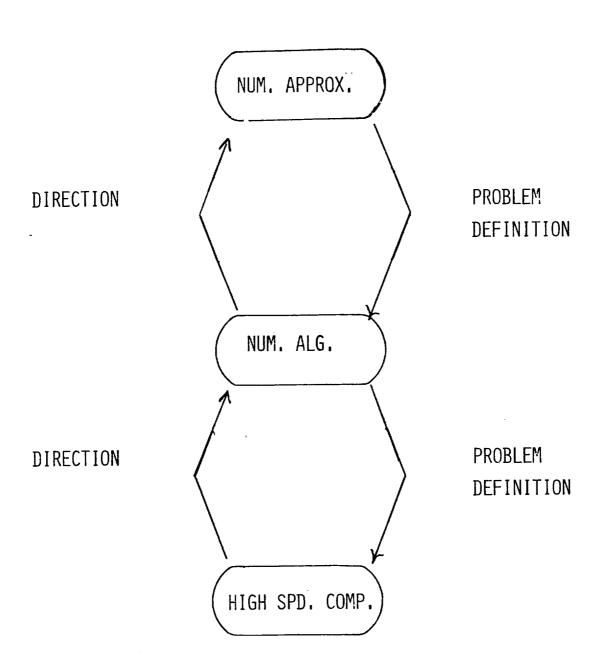


USE VECTOR REGISTERS AS TEMPORARY STORAGE

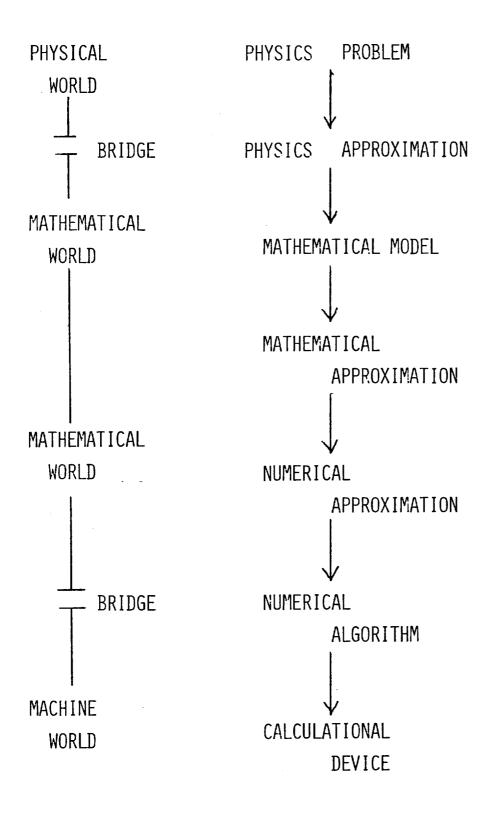


KEY POINTS TO REMEMBER

- VECTOR COMPUTER HAS GENERATED A NEW MATHEMATICAL TOOL
 FOR THE NUMERICAL ANALYST
- MORE MATHEMATICAL THEORY NEEDS TO BE DEVELOPED
- COMPILERS CANNOT GENERATE THE OPTIMAL ALGORITHM
- MANY NEW ALGORITHMS HAVE BEEN DEVELOPED



RECALL: THE SCIENTIFIC COMPUTATIONAL PROCESS

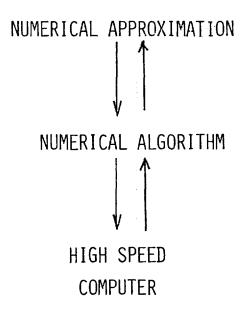


MAIN DIFFICULTY IN NUMERICAL ALGORITHM DEVELOPMENT: COMMUNICATION PROBLEMS

RESEARCH AREAS	PHYSICIST	MATH.	COMP. SCI.
MESEANOT ANEAS			COHE, SCI.
PHYSICS PROBLEM		! !	
PHYSICS APPROXIMATION		 	
		; .}	
MATHEMATICAL MODEL			
MATHEMATICAL APPROXIMATION			
NUMERICAL APPROXIMATION		·	
NUMERICAL ALGORITHM			i ! !
HIGH SPEED COMPUTER		 	
COMP. SCI. AREAS			

THE BASIC GOAL OF THE EFFORT IN NUMERICAL ALGORITHMS:

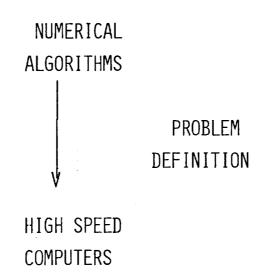
MAKE THIS LINK IN COMPUTATIONAL PROCESS AS STRONG AS POSSIBLE



BY

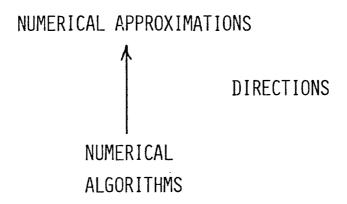
- 1) RESEARCH IN NUMERICAL ALGORITHMS
- 2) PROBLEM DEFINITION TO HIGH SPEED COMPUTER ARCHITECTS
- 3) FOCUS RESEARCH IN NUMERICAL APPROXIMATIONS

OTHER ACTIVITIES



- GENERATING LARGE SCALE COMPUTER CODES FOR RESEARCH PURPOSES BY
 - ACADEMIC
 - INDUSTRY
 - LABORATORY
- THESE CODES WILL CONTAIN ALGORITHMS GENERATED FROM RESEARCH

OTHER ACTIVITIES



- NEW TIME-DIFFERENCING TECHNIQUES HAVE BEEN DEVELOPED
- NEW RESULTS IN CONJUGATE GRADIENT METHOD

CONCLUDING REMARKS

- COMPUTERS DO INFLUENCE THE TYPE OF NUMERICAL
 ALGORITHMS THAT ARE USED IN YOUR CALCULATION
- NUMERICAL ALGORITHMS ARE THE BRIDGE BETWEEN
 THE PHYSICAL WORLD AND THE COMPUTING MACHINE
 DON'T TRY TO BY-PASS THEM
- TALK TO YOUR FRIENDLY NUMERICAL ANALYST. THEY
 CAN REALLY HELP YOU TO
 - 1) BUILD A BETTER COMPUTER
 - 2) SOLVE YOUR PROBLEM ON AN EXOTIC COMPUTER